NERL/AMD Publications

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ABSTRCT/ORAL

Singh, R.B., Huber, A.H., and Braddock, J.N. Development of real-time site-specific microscale emission factor model for the assessment of human exposure to motor vehicle emissions. Presented at: 11th Coordinating Research Council On-Road Vehicle Emissions Workshop, San Diego, CA, March 26-28, 2001. 3/26/2001

Contact: Alan H. Huber

Abstract: The United States Environmental Protection Agency's (EPA) National Expsoure Research Laboratory (NERL) has initiated a project to improve the methodology for modeling urban-scale human exposure to mobile source emissions. The modeling project has started by considering the need for an emission model that is structured to support human exposure assessment. Current emission models have not been designed to estimate real-time emissions needed to support human exposure studies near roadways. Disaggregated real-time emission factors are needed for roadway dispersion and human exposure modeling in specific microenvironments. The MicroFac models are being developed from existing databases using new modeling approaches suitable for microscale modeling. This presentation summarizes progress on the model development and example applications.

JOURNAL

Xiu, A., and Pleim, J.A. Development of a land-surface model part I: application in a mesoscale meteorology model. February 2001. Journal of Applied Meteorology 40 (2):192-209 (2001). EPA/600/J-01/266. 9/4/2001

Contact: Jonathan A. Pleim

Abstract: Parameterization of land-surface processes and consideration of surface inhomogeneities are very important to mesoscale meteorological modeling applications, especially those that provide information for air quality modeling. To provide crucial, reliable information on the diurnal evolution of the planetary boundary layer (PBL) and its dynamic characteristics, it is necessary in a mesoscale model to include a land surface parameterization that simulates the essential physics processes and is computationally efficient. A land surface model is developed and implemented in the Fifth Generation Penn State/NCAR Mesoscale Model (MM5) to enable MM5 to respond to changing soil moisture and vegetation conditions. This land surface model includes explicit soil moisture, which is based on the Interaction Soil Biosphere Atmosphere (ISBA) model and three pathways for evaporation including soil evaporation, canopy evaporation, and vegetative evapotranspiration. The stomatal conductance, leaf to canopy scaling, and surface moisture parameterizations are newly developed based on a variety of sources in the current literature. Also, a processing procedure for gridding soil and vegetation parameters and simulating seasonal growth has been developed. MM5 with the land surface model is tested and evaluated against observations and the "standard" MM5, which uses a simple surface moisture availability scheme to estimate the soil wetness then the latent heat flux, for two cases from the First International Satellite Land Surface Climatology Project Field Experiment (FIFE). The evaluation analysis focuses primarily on surface fluxes of heat and moisture, near surface temperature, soil temperature, PBL height, and vertical temperature profiles. A subsequent article will describe extensions of this model to simulate chemical dry deposition. The U.S. Environmental Protection Agency through its Office of Research and Development funded the research described here under cooperative agreement CR-823628 to the MCNC-Environmental Programs. It has been subjected to agency review and approved for publication. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

Singh, R.B., Huber, A.H., and Braddock, J.N. Sensitivity analysis and evaluation of microfaco: a microscale motor vehicle emission factor model for CO emissions. Journal of the Air & Waste Management Association 51 (7):1087-1099 (2001). EPA/600/J-01/237. 6/1/2001

Contact: Alan H. Huber

Abstract: The United States Environmental Protection Agency's National Exposure Research Laboratory has initiated a project to improve the methodology for modeling human exposure to motor vehicle emissions. The overall project goal is to develop improved methods for modeling the source through the air pathway to human exposure in significant microenvironments of exposure. The PART models (used in the United States, except California) and EMFAC models (used in California only) used to estimate emissions are suitable only for regional (county) scale modeling and emission inventories because of their dependence on aggregated vehicle-miles-traveled data. These emission models are not designed to estimate real-time emissions needed for human exposure studies near roadways. Therefore, there is a need to develop site-specific real-time emission factor models for PM emissions. A microscale emission factor model for predicting site-specific real-time motor vehicle particulate matter (MicroFacPM) emissions for TSP, PM10 and PM2.5 has been developed. It uses site-specific available information on the vehicle fleet composition. The algorithm used to calculate emission factors in MicroFacPM is disaggregated based on the site-specific vehicle fleet. The emission factors are calculated from a real-time fleet, rather than from a fleet-wide average estimated by a vehicle-miles-traveled weighting of the emission factors for different vehicle classes. MicroFacPM requires input information necessary to characterize the site-specific real-time fleet being modeled. Other variables required are average vehicle speed, time and day of the year, ambient temperature and relative humidity. The U.S. Environmental Protection Agency through its Office of Research and Development funded the research described here. This manuscript has been subjected to Agency review and approval for publication. Mention of trade names or commercial products does not constitute an endorsement or recommendation for use.

PUB REPORT

Atmospheric Modeling Division, and EPA Systems Development Center. Models-3 installation procedures for a sun workstation with a unix-based operating system (Models-3 Version 4.1). 2001. EPA/600/R-01/037 (NTIS PB2002-107934) , http://www.epa.gov/asmdnerl/models3/. 6/4/2001

Contact: William G. Benjey

Abstract: Models-3 is a flexible system designed to simplify the development and use of air quality models and other environmental decision support tools. It is designed for applications ranging from regulatory and policy analysis to understanding the complex interactions of atmospheric chemistry and physics. The May 2001 release of Models-3 contains a Community Multi-scale Air Quality (CMAQ) modeling system for urban to regional scale air quality simulation of tropospheric ozone, acid deposition, visibility, and fine particles. The major improvements in CMAQ since the June 2000 release include the Modified Euler Backward Iterative (MEBI) chemical solver for use with CB4 gas-phase mechanisms, improved horizontal diffusion, and an improved aerosol module. Principal changes to other parts of the Models-3 system improvements include the replacement of the former emission modeling system with provision to use the Sparse Matrix Operator Kernel Emission (SMOKE) modeling system (available at no cost from MCNC, North Carolina Supercomputing Center), and a SMOKE Tool to create input files for SMOKE. This Installation Manual includes an overview of the system architecture, installation requirements, procedures for installation of the Models-3 server and clients, establishing users, Models-3 start-up and shut-down, loading of data sets, description of system administration functions, and illustrative examples. Release notes describing system changes (including SMOKE Tool) are in Appendices G and H. This updated installation and operation manual is a part of the documentation set for the Models-3 Third Generation Air Quality Modeling System. The U.S. Environmental Protection Agency through its Office of Research and Development partially funded and collaborated in the procedures described here under contracts 68-W1-0055 and 68-W-99-002 to Science Applications International Corporation. This Manual has been subjected to the Agency's peer and administrative review and has been approved for publication as an EPA document. Mention of trade names or commercial products is not intended to constitute endorsement or recommendation for use.

Atmospheric Modeling Division, and EPA Systems Development Center. SMOKE tool for Models-3 version 4.1 structure and operation documentation. 2001. EPA/600/R-01/048 (NTIS PB2001-108312) , http://www.epa.gov/asmdnerl/models3/. 8/2/2001

Contact: William G. Benjey

Abstract: The SMOKE Tool is a part of the Models-3 system, a flexible software system designed to simplify the development and use of air quality models and other environmental decision support tools. The SMOKE Tool is an input processor for SMOKE, (Sparse Matrix Operator Kernel Emission system) the air emission modeling component of Version 4.1 of Models-3. The SMOKE Tool provides emission file in the correct format, creates gridded files of emission data, and performs quality control and analysis of emission data for SMOKE. SMOKE Tool may be operated either within the graphical user interface of Models-3 system, or independently in a "stand-alone" mode. SMOKE Tool is made available with a set of standard EPA emission inventories for the years 1990, 1995, and 1996 as well as economic projection factors and temporal and spatial allocation data. This document provides detailed descriptions of the software structure, related file formats and assumptions, environment variable settings, and other details for the use of SMOKE Tool. SMOKE Tool and this document are available from the Models-3 web site at http://www.epa.gov/asmdnerl/models3/. This document has been subjected to the Agency's peer and administrative review and has been approved for publication as an EPA document. Mention of trade names or commercial products is not intended to constitute endorsement or recommendation for use.

Atmospheric Modeling Division, and EPA Systems Development Center. Models-3 installation procedures for a personal computer with a NT operating system (Models-3 version 4.1). 2001. EPA/600/R-01/046 (NTIS PB2002-100445) , http://www.epa.gov/models3/. 9/21/2001

Contact: William G. Benjey

Abstract: Models-3 is a flexible system designed to simplify the development and use of air quality models and other environmental decision support tools. It is designed for applications ranging from regulatory and policy analysis to understanding the complex interactions of atmospheric chemistry and physics. The 2001 release of Models-3 contains a Community Multi-Scale Air Quality (CMAQ) modeling system for urban to regional scale air quality simulation of tropospheric ozone, acid deposition, visibility, and fine particles. The major improvements in CMAQ since the June 2000 release include the Modified Euler Backward Iterative (MEBI) chemical solver for use with CB4 gas-phase mechanisms, improved horizontal diffusion, and an improved aerosol module. Principal changes to other parts of the Models-3 system improvements include the replacement of the former emission modeling system with provision to use the Sparse Matrix Operator Kernel Emission (SMOKE) modeling system (available at no cost from MCNC, North Carolina Supercomputing Center), and SMOKE Tool to create input files for SMOKE. This Installation Manual is for both new installations and upgrades, and includes an overview of the Models-3 server and clients, establishing users, Models-3 start-up and shut-down, loading of data sets, description of system administration functions, and illustrative examples. Release notes describing changes (including SMOKE Tool) are in the Appendices.

Atmospheric Modeling Division, and EPA Systems Development Center. Release notes for Models-3 version 4.1 patch: SMOKE tool and file converter. 2001. EPA/600/R-01/076 (NTIS PB2002-101194) , http://www.epa.gov/asmdnerl/models3/. 10/3/2001

Contact: William G. Benjey

Abstract:

SYMPOS/CONF

Ching, J.K.S., Lacser, A., Byun, D.W., and Benjey, W.G. "Air quality modeling at neighborhood scales to improve human exposure assessment." Paper presented at: Third International Conference on Urban Air Quality, Loutraki, Greece, March 19-23, 2001. 3/19/2001

Contact: Jason K. Ching

Abstract:

Godowitch, J.M. Results of photochemical simulations of subgrid scale point source emissions with the Models-3 CMAQ modeling system. Presented at: Millenium Symposium on Atmospheric Chemistry, Albuquerque, NM, January 14-19, 2001. EPA/600/A-00/114 (NTIS PB2001-101918). 1/14/2001

Contact: James M. Godowitch

Abstract: The Community Multiscale Air Quality (CMAQ) / Plume-in-Grid (PinG) model was applied on a domain encompassing the greater Nashville, Tennessee region. Model simulations were performed for selected days in July 1995 during the Southern Oxidant Study (SOS) field study program which was conducted in the Nashville area. In particular, five major point sources exhibiting a range of Nox emission rates were selected for the PinG treatment. Selected PinG model concentrations and representative examples of the initial results of an ongoing evaluation of the PinG model with the SOS/Nashville data are presented to provide a preliminary demonstration of the capability of the CMAQ/PinG approach. In particular, modeled concentrations of ozone, SO2, and nitrogen oxides are compared to plume data collected during horizontal traverses by an instrumented helicopter and research aircraft across different plumes. Statistical results are also provided at 40 km downwind of the largest point source. The comparisons and quantitative results are encouraging as PinG exhibited the capability to realistically simulate the observed photochemical evolution for ozone and other species at various downwind distances for these cases.

Eder, B.K., LeDuc, S.K., Gilliland, A.B., and Finkelstein, P.L. On the use of NEXRAD stage IV data in the multimedia modeling of pollutant transport. Presented at: Symposium on Precipitation Extremes: Prediction, Impacts, and Responses, Boston, MA, January 14-19, 2001. EPA/600/A-00/115 (NTIS PB2001-101919). 1/14/2001

Contact: Brian K. Eder

Abstract:

Otte, T.L., and Lacser, A. Implementation of an urban canopy parameterization in MM5 for meso-gamma-scale air quality modeling applications. Presented at: Proceedings AMS Ninth Conference on Mesoscale Processes, Ft. Lauderdale, FL, July 30-August 2, 2001. 7/30/2001

Contact: Tanya L. Otte

Abstract: The U.S. Environmental Protection Agency (U.S. EPA) is extending its Models-3/Community Multiscale Air Quality (CMAQ) Modeling System to provide detailed gridded air quality concentration fields and sub-grid variability characterization at neighborhood scales and in urban areas. CMAQ is an advanced air quality modeling system that embodies a "one-atmosphere," multiple-pollutant philosophy (Byun and Ching, 1999). There are three primary models within Models-3/CMAQ: meteorology, emissions, and chemistry. The meteorology model used with CMAQ in this application is the Pennsylvania State University/National Center for Atmospheric Research (PSU/NCAR) Mesoscale Model (MM5; Grell et al. 1994). For fine-scale urban simulations (~1-km grid spacing), MM5 has been modified to include an urban canopy parameterization that accounts for drag exerted by the urban structures, the enhancement of turbulent kinetic energy (especially near the top of the buildings), and the energy budget at the street and roof levels. This refinement of MM5 is targeted to provide CMAQ with the means to capture the details of pollutant spatial distributions at these scales. One of the goals of this research is to demonstrate the capability of MM5 to simulate the effects of urban areas at the meso-gamma scale. This paper describes the suggested modifications to MM5 and presents preliminary results of using the urban canopy parameterization. The information in this manuscript has been funded by the United States Environmental Protection Agency. It has been subjected to Agency review and approved for publication. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

Eder, B.K., Mebust, M.R., and LeDuc, S.K. A preliminary evaluation of Models-3 CMAQ using particulate matter data from the IMPROVE network. Presented at: 25th NATO/CCMS International Technical Meeting on Air Pollution Modeling and Its Application, Louvain-la-Neuve, Belgium, October 15-19, 2001. EPA/600/A-01/076 (NTIS PB2002-100287). 10/15/2001

Contact: Brian K. Eder

Abstract: The Clean Air Act and its Amendments require the United States Environmental Protection Agency (EPA) to establish National Ambient Air Quality Standards for Particulate Matter (PM) and to assess current and future air quality regulations designed to protect human health and welfare. Air quality models, such as EPA's Models-3 Community Multiscale Air Quality model (CMAQ) [Byun and Ching, 1999], provide one of the most reliable tools for performing such assessments. CMAQ simulates air concentrations and deposition of various pollutants including PM. These simulations, which can be conducted on a myriad of spatial and temporal scales, support both regulatory assessment as well as scientific studies by research institutions. Within CMAQ is an aerosol component, or module, designed to simulate the complex processes involving PM, which is commonly separated into PM2.5 and PM10. In order to determine its value to the air quality regulatory communities, CMAQ needs to be evaluated using observational data. One such evaluation, which compared visibility parameters derived from CMAQ to visibility parameters obtained from National Weather Service observations, revealed that CMAQ was able to replicate general spatial and temporal patterns [Eder et al., 2000]. The current evaluation compares PM simulated by CMAQ with PM data collected by the Interagency Monitoring of PROtected Visual Environments (IMPROVE) network.

Ching, J.K.S. Modeling air toxics and PM 2.5 concentration fields as a means for facilitating human exposure assessments. Presented at: Proceedings of the 10th International Symposium Transport and Air Pollution, Boulder, CO, September 17-19, 2001. EPA/600/A-01/077 (NTIS PB2002-100286). 9/17/2001

Contact: Jason K. Ching

Abstract: The capability of the US EPA Models-3/Community Multiscale Air Quality (CMAQ) modeling system is extended to provide gridded ambient air quality concentration fields at fine scales. These fields will drive human exposure to air toxics and fine particulate matter (PM2.5) models, and ultimately influence implementation of ambient air quality regulatory standards. Sub-grid variability of the pollutant distribution serves as ancillary information for exposure assessments and "hot-spot" analyses to assess impacts of various sources of air toxic pollutants. This paper describes the modeling enhancements to the existing CMAQ, as well as the strategy we are exploring to provide the sub-grid scale details that fulfill the proposed model design requirements and functionality. The information in this manuscript has been prepared under funding by the United States Environmental Protection Agency. It has been subjected to Agency review and approved for publication. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

Pleim, J.A., and Xiu, A. Updates and evaluation of the PX-LSM in MM5. Presented at: MM5 Users Workshop, Boulder, CO, June 25-27, 2001. EPA/600/A-01/082 (NTIS PB2002-100285). 6/25/2001

Contact: Jonathan A. Pleim

Abstract: Starting with Version 3.4, there is a new land surface model known as the Pleim-Xiu LSM available in the MM5 system. Pleim and Xiu (1995) described the initial development and testing of this land surface and workshop proceedings provided a basic description of the model and some evaluation (Pleim and Xiu, 2000). A recent journal article (Xiu and Pleim, 2001) presents a more detailed description of the LSM and its implementation in MM5 and further evaluation. This paper outlines some bug fixes, updates, guidance for use, and more evaluation. This paper has been reviewed in accordance with the US Environmental Protection Agency's peer and administrative review policies and approved for presentation and

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Presented *Published*

Huber, A.H., Freeman, M., Rida, S., Kuehlert, K.H., and Bish, I.E.S. "Development and applications of CFD in support of air quality studies of roadway and building microenvironments." Paper presented at: 94th AWMA Conference, Orlando, FL, June 24-28, 2001. 6/24/2001

Contact: Alan H. Huber

Abstract: There is a need to develop modeling and data analysis tools to increase our understanding of human exposures to air pollutants beyond what can be explained by "limited" field data. Modeling simulations of complex distributions of pollutant concentrations within roadway and building microenvironments is feasible using high performance computing. Output from high performance computing can both be directly used to better understand specific exposure events and used to develop better simplified model approximations that may be generally applied. Unlike most currently used regulatory air quality models, Computational Fluid Dynamics (CFD) simulations are able to account rigorously for topographical details such as terrain variations and building structures in urban areas as well as local aerodynamics and turbulence. This paper discusses the development and application of CFD simulations through case studies using Fluent, Inc. Computational Fluid Dynamics software for simulating air pollutant concentrations from sources near roadways and buildings. Comparisons of CFD simulations to both wind tunnel and field measured wind and pollutant concentrations are bing used to provide evaluation/validation examples that document the reliability and accuracy of Fluent's existing CFD software. This paper presents a report on progress. The U.S. Environmental Protection Agency through its Office of Research and Development funded the research described here. It has been subjected to Agency review and approved for publication. Mention of trade names or commercial products does not constitute an endorsement or recommendation for use.

Singh, R.B., Huber, A.H., and Braddock, J.N. Development of a microscale emission factor model for particulate matter (MicroFacPM) for predicting real-time motor vehicle emissions. Presented at: 94th AWMA Conference, Orlando, FL, June 24-28, 2001. EPA/600/A-01/034. 6/24/2001

Contact: Alan H. Huber

Abstract: The United States Environmental Protection Agency's National Exposure Research Laboratory has initiated a project to improve the methodology for modeling human exposure to motor vehicle emissions. The overall project goal is to develop improved methods for modeling the source through the air pathway to human exposure in significant microenvironments of exposure. The PART models (used in the United States, except California) and EMFAC models (used in California only) used to estimate emissions are suitable only for regional (county) scale modeling and emission inventories because of their dependence on aggregated vehicle-miles-traveled data. These emission models are not designed to estimate real-time emissions needed for human exposure studies near roadways. Therefore, there is a need to develop site-specific real-time emission factor models for PM emissions. A microscale emission factor model for predicting site-specific real-time motor vehicle particulate matter (MicroFacPM) emissions for TSP, PM10 and PM2.5 has been developed. It uses site-specific available information on the vehicle fleet composition. The algorithm used to calculate emission factors in MicroFacPM is disaggregated based on the site-specific vehicle fleet. The emission factors are calculated from a real-time fleet, rather than from a fleet-wide average estimated by a vehicle-miles-traveled weighting of the emission factors for different vehicle classes. MicroFacPM requires input information necessary to characterize the site-specific real-time fleet being modeled. Other variables required are average vehicle speed, time and day of the year, ambient temperature and relative humidity. The U.S. Environmental Protection Agency through its Office of Research and Development funded the research described here. This manuscript has been subjected to Agency review and approval for publication. Mention of trade names or commercial products does not constitute an endorsement or recommendation for use.

Presented *Published*

Dennis, R.L., Tonnesen, G.S., and Mathur, R. "Nonlinearities in the sulfate secondary fine particulate response to NOx emissions reductions as modeled by the regional acid deposition model." Paper presented at: Millennium NATO/CCMS International Technical Meeting on Air Pollution Modeling and Its Application, Boulder, CO, May 15-19, 2000. 5/14/2001

Contact: Robin L. Dennis

Abstract: Attention is increasingly being devoted to the health effects of fine particulates. In regions that have a large production of sulfate, sulfuric acid and nitric acid compete for the available ammonia to form aerosols. In addition, the available nitric acid is the result of urban and regional photochemical production, as are the oxidant fields involved in the oxidation of SO2 to sulfate. To create an integrated modeling capability to investigate the particulate cycling, the Regional Acid Deposition Model (RADM) was enhanced by adding several modules to dynamically represent the physical and chemical processes involved in the geochemical cycling of sulfate and reduced and oxidized forms of nitrogen. The modules are based on those of the Regional Particulate Model (RPM); the resulting version of the model is referred to as the Extended RADM. The Extended RADM is used to investigate the connection between oxidant production and secondary particulate production resulting from NOx-SOx-NHx interactions. The reduction of regional NOx emissions from major point sources has been proposed as a means to reduce levels of regional and urban ozone. Many thought the overall level of sulfate and nitrate fine particulate, and the associated ammonium, would decrease for these emissions reductions. The effect on secondary fine particulate levels resulting from a reduction in regional NOx emissions for the eastern United States was investigated with the Extended RADM. It was found that in parts of the domain, but not everywhere, the fine particulate mass increased due to increases in sulfate. In different parts the reason for the increase was different. Around a few cities the increase in OH associated with the NOx - Ozone disbenefit was the cause. In western Pennsylvania, the increase in hydrogen peroxide due to increased radical termination was the cause. The nonlinear increase in fine particle mass due to a reduction in NOx emissions is explainable through the examination of the response in different chemical regimes.

LeDuc, S.K. Supporting the data needs of the coastal community II: Hurricane Floyd post-event. Presented at: 17th Conference on Interactive Information and Processing Systems for Meteorology, Oceanography, and Hydrology, Boston, MA, January 14-19, 2001. EPA/600/A-00/113 (NTIS PB2001-101917). 1/14/2001

Contact: Sharon K. Leduc

Abstract:

Benjey, W.G., Houyoux, M.R., and Susick, J.W. Implementation of the SMOKE emission data processor and SMOKE tool input data processor in Models-3. Presented at: The Emission Inventory Conference, Denver, CO, May 1-4, 2001. EPA/600/A-01/027 (NTIS PB2001-104620). 5/1/2001

Contact: William G. Benjey

Abstract: The U.S. Environmental Protection Agency has implemented Version 1.3 of SMOKE (Sparse Matrix Object Kernel Emission) processor for preparation of area, mobile, point, and biogenic sources emission data within Version 4.1 of the Models-3 air quality modeling framework. The SMOKE system includes MOBILE 5b to model on-road emissions and the Biogenic Emission Inventory System, Version 2 (BEIS 2) to model biogenic emissions. Although SMOKE may be operated from scripts outside of the Models-3 framework, integration within the system allows automatic registration and tracking of input and output files, as well as close coupling to the Community Multiscale Air Quality (CMAQ) modeling system and visualization tools by using the Net CDF I/O API data format convention. Models-3 also includes the SMOKE Tool to assist in preparation of emission input data for SMOKE. The SMOKE Tool performs basic functions for the user, including 1) import and quality checking of emission inventory and related data, 2) preparation of user-defined model grids and gridding of emission data and surrogates (SMOKE Tool requires a Geographic Information System (GIS), 3) preparation of user-defined "packet" files which instruct SMOKE to apply factors including growth, control, and reactivity analysis factors (individual species may be added or deleted by source and location), and 4) allows the user to edit input files. Manual preparation of input files outside of the system is possible, but increases the probability of human error and substantially increases the time needed for data preparation.